

Electronic correlations and flattened band in magnetic Weyl semimetal $\text{Co}_3\text{Sn}_2\text{S}_2$

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The interplay between electronic correlations and topological protection may offer a rich avenue for discovering emergent quantum phenomena in condensed matter. However, electronic correlations have so far been little investigated in Weyl semimetals (WSMs) by experiments. Here, we report a combined optical spectroscopy and theoretical calculation study on the strength of electronic correlations in a kagome magnet $\text{Co}_3\text{Sn}_2\text{S}_2$ and the influence of electronic correlations on its WSM state expected within a single-particle picture. The electronic kinetic energy estimated from our optical data is about half of that obtained from single-particle *ab initio* calculations, which indicates intermediate-strength electronic correlations in this system. Furthermore, comparing the energy ratios between the interband-transition peaks at high energies in the experimental and single-particle-*ab-initio*-calculation-derived optical conductivity spectra with the electronic-bandwidth renormalization factors obtained by many-body calculations enables us to estimate the Coulomb-interaction strength ($U \sim 4$ eV) of electronic correlations in $\text{Co}_3\text{Sn}_2\text{S}_2$. Our many-body calculations with $U \sim 4$ eV show that a WSM state, which is characterized by bulk Weyl cones and surface Fermi arcs, survives in this correlated electron system. More importantly, a sharp experimental optical conductivity peak at low energy, which is absent in the single-particle-*ab-initio*-calculation-derived optical conductivity spectrum but is consistent with the optical conductivity peaks obtained by many-body calculations, indicates that an electronic band connecting the two Weyl cones is flattened by electronic correlations and emerges near the Fermi energy in $\text{Co}_3\text{Sn}_2\text{S}_2$. Our work not only provides a paradigm for identifying WSM phase in correlated materials, but also paves the way for exploring flat-band-generated quantum phenomena in WSMs.

Electronic correlations, which is a type of many-body interactions—Coulomb interactions between electrons, lie at the heart of condensed matter physics due to their crucial roles in producing a variety of novel quantum phenomena, such as unconventional superconductivity [1, 2], heavy-fermion behavior [3, 4], and Mott insulation [5]. Thus, theoretical predictions and experimental observations of topological quantum states in real materials with significant electronic correlations have generated tremendous interest in the scientific community [6–9]. Therein, Weyl semimetals (WSMs) represent a kind of topological quantum states which host pairs of bulk Weyl cones and surface Fermi arcs connecting pairs of Weyl points with opposite chirality [9–19]. Recently, theoretical studies indicate that sufficiently strong elec-

tronic correlations can gap out bulk Weyl nodes and thus break WSM states [20–30]. Therefore, it is significant to further investigate whether a WSM state predicted in a non-interacting single-particle picture still exists in the presence of electronic correlations [31–35]. Additionally, several correlated electron systems, such as kagome-lattice compounds [36, 37] and heavy-fermion materials [38], have been reported to host flat bands (i.e., dispersionless bands) which can provide a footstone for the emergence of various quantum phenomena, including superconductivity [39, 40], ferromagnetism [41, 42] and fractional quantum Hall effect [43–46]. Nonetheless, electronic-correlation-induced flat bands have rarely been observed in WSMs. Lately, single-particle *ab initio* predictions of WSM states in 3d-transition-metal com-

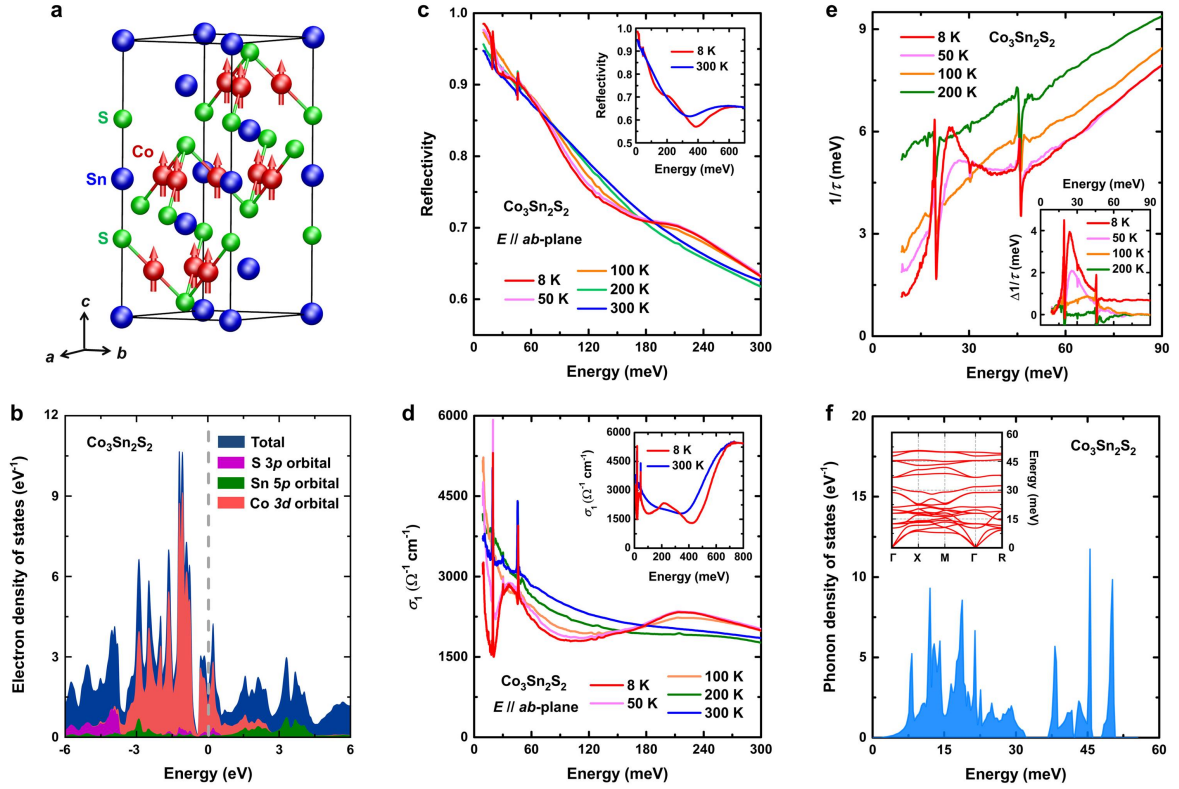


FIG. 1: **Ab-plane optical response of $\text{Co}_3\text{Sn}_2\text{S}_2$.** **a**, Crystal structure of $\text{Co}_3\text{Sn}_2\text{S}_2$. A quasi-two-dimensional Co_3Sn layer is sandwiched between the sulfur atoms. The magnetic moments on the cobalt sites are along the c -axis. **b**, Electron density of states (DOS) obtained by single-particle *ab initio* calculations. The electron DOS near the Fermi energy is mainly contributed by the electronic bands with Co 3d orbital characters. **c**, Several representative reflectance spectra $R(\omega)$ measured with the electric field (E) of the incident light parallel to the crystalline ab -plane. The inset shows that the $R(\omega)$ up to 700 meV. **d**, Real parts $\sigma_1(\omega)$ of the ab -plane optical conductivity at different temperatures. The inset displays the $\sigma_1(\omega)$ up to 800 meV. **e**, Electronic scattering rate spectra $1/\tau(\omega)$. The inset shows the relative scattering rate spectra $\Delta 1/\tau(\omega)$ obtained by subtracting the linear backgrounds. A hump-like feature is present around 24.3 meV in the $\Delta 1/\tau(\omega)$ when the temperature is lower than the FM transition temperature $T \sim 177$ K. **f**, Phonon density of states obtained by *ab initio* calculations. The inset depicts the calculated phonon dispersions. The phonon DOS and the phonon dispersions are cut off at ~ 50.8 meV.

pounds shed light on searching for correlated WSMs with flat bands, owing to the intimate association between the weak spatial extension of 3d orbitals and large Coulomb interactions [47–50].

A cobalt-based shandite compound, $\text{Co}_3\text{Sn}_2\text{S}_2$, crystallizes in a rhombohedral structure with the cobalt atoms forming a kagome lattice within one quasi-two-dimensional Co_3Sn layer (see Fig. 1a) and exhibits long-range ferromagnetic (FM) order with a magnetic moment of $\sim 0.3 \mu_B$ (μ_B denotes the Bohr magneton) per cobalt atom below temperature $T \sim 177$ K [51–54]. Single-particle *ab initio* calculations show that the electronic bands of FM $\text{Co}_3\text{Sn}_2\text{S}_2$ near the Fermi energy (E_F) are dominated by cobalt 3d orbitals (see the electron density of states (DOS) for $\text{Co}_3\text{Sn}_2\text{S}_2$ with the Co 3d, Sn 5p and S 3p orbital contributions shaded in red, green and purple colors, respectively in Fig. 1b) [37], but the strength of electronic correlations in this FM 3d-transition-metal compound remains unclear. Furthermore, single-particle *ab initio* calculations suggest that FM $\text{Co}_3\text{Sn}_2\text{S}_2$ is a con-

tender for magnetic WSMs [47–49]. Up to now, important progresses in the experimental studies of the predicted WSM state in FM $\text{Co}_3\text{Sn}_2\text{S}_2$, which involve the measurements of negative magnetoresistance, giant intrinsic anomalous Hall and Nernst effects [47, 49, 55, 56], have been achieved. However, as two fingerprints of a WSM state, Weyl cones in the bulk and Fermi arcs on the surface have seldom been observed in FM $\text{Co}_3\text{Sn}_2\text{S}_2$. Therefore, if electronic correlations have nonnegligible effects on the electronic properties of this system, further investigations, which take into account electronic correlations, will be needed to check whether a WSM state persists in FM $\text{Co}_3\text{Sn}_2\text{S}_2$. Moreover, the influence of electronic correlations on the single-particle-*ab-initio*-calculation-derived WSM state in this WSM candidate, for example, inducing a flat band, remains elusive.

Results

Reduction of the electronic kinetic energy. Optical spectroscopy is a bulk-sensitive experimental technique

for studying charge dynamics and electronic band structure of a material as it probes both itinerant charge carriers and interband transitions from occupied to empty states [64–69]. Here, to investigate electronic correlations and their effects on the previously predicted WSM state in FM $\text{Co}_3\text{Sn}_2\text{S}_2$, we measured the optical reflectance spectra $R(\omega)$ of its single crystals at low temperatures with the electric field (E) of the incident light parallel to the crystalline ab -plane over a broad photon energy (ω) range (see the details about the reflectance measurements and the sample growth in Methods section). Figure 1c depicts the $R(\omega)$ of $\text{Co}_3\text{Sn}_2\text{S}_2$ single crystals measured at different temperatures. The $R(\omega)$ at energies lower than 20 meV not only approach to unity, but also increase as the temperature decreases, which exhibits the optical response of a metal. Moreover, the real parts (i.e., $\sigma_1(\omega)$) of the ab -plane optical conductivity of $\text{Co}_3\text{Sn}_2\text{S}_2$ in Fig. 1d, which were obtained by the Kramers-Kronig transformation of the $R(\omega)$ (see Methods section), show Drude-like features of metals at energies lower than 20 meV. The Drude-like features in the low-energy parts of the $\sigma_1(\omega)$ and the fast-increasing value of the $R(\omega)$ at low energies indicate the existence of itinerant charge carriers in $\text{Co}_3\text{Sn}_2\text{S}_2$, which provides an opportunity for studying the electronic correlation effect on the motion of the itinerant charge carriers. Furthermore, several peak-like features arising from interband transitions are present in the high-energy parts of the $\sigma_1(\omega)$. A comparison between the experimental interband-transition energies determined via the optical measurements and the theoretical interband-transition energies calculated without considering electronic correlations enables us to gain insights into the effect of electronic correlations on the bandwidth.

To provide an overview of the possible many-body interactions in FM $\text{Co}_3\text{Sn}_2\text{S}_2$, we extracted its electronic scattering rate spectra $1/\tau(\omega)$ by performing the extended Drude analysis of the optical data [64–66, 69] (see Methods section). The $1/\tau(\omega)$ at different temperatures were plotted in Fig. 1e. Interestingly, when the temperature is lower than the FM phase transition temperature $T \sim 177$ K, a hump-like feature emerges around 24.3 meV in the relative electronic scattering rate spectra $\Delta 1/\tau(\omega)$ obtained by subtracting the linear backgrounds (see the inset of Fig. 1e and Fig. S1 of Supplementary Information). The presence of hump-like feature in the FM state implies that a strong scattering channel, which is intimately associated with the interactions between the ferromagnetically ordered spins (i.e., ordered spin-spin correlations), may appear with the formation of the low-temperature long-range FM order in $\text{Co}_3\text{Sn}_2\text{S}_2$. Moreover, three dip-like features, which correspond to the three infrared-active phonon peaks in the $\sigma_1(\omega)$, can be observed in the $1/\tau(\omega)$ at $\omega \approx 19.7$, 30.1 and 46.2 meV, respectively. Since (i) electron-phonon coupling usually results in an energy-independent scattering rate above the upper limit of phonon energies [64], and (ii)

our single-particle *ab initio* calculations show that the phonon dispersions and the phonon density of states are cut off at ~ 50.8 meV (see Fig. 1f and the calculation details in Methods section), the approximately linear energy dependence of the $1/\tau(\omega)$ in the energy range from 51 to 90 meV suggests that besides electron-phonon scattering, other scattering channels coming from other many-body interactions, like electronic correlations and spin-spin correlations, exist in $\text{Co}_3\text{Sn}_2\text{S}_2$. Then, a question naturally arises: which type of many-body interactions plays a dominant role in affecting the motion of the itinerant charge carriers and the width of the electronic bands in this magnetic WSM candidate?

To gain insights into this question, we firstly compare the experimentally measured kinetic energy with the theoretical kinetic energy calculated without taking any many-body interaction into account. Following the definition of the electronic kinetic energy in the optical study of a multiband system LaOFep [66], we can obtain the linear relationship between the electronic kinetic energy (K) and the spectral weight (S) of the Drude component (i.e., the area under the Drude component) of the $\sigma_1(\omega)$:

$$K = \frac{2\hbar^2 d_0}{\pi e^2} S = \frac{2\hbar^2 d_0}{\pi e^2} \int_0^{\omega_c} \sigma_1(\omega) d\omega, \quad (1)$$

where ω_c is a cut-off energy for integrating the Drude component of the $\sigma_1(\omega)$, \hbar is Planck's constant divided by 2π , e is the elementary charge and d_0 is the inter- Co_3Sn -layer distance. Figure 2a displays the Drude components of the real part of the experimental optical conductivity $\sigma_1^E(\omega)$ at $T = 8$ K and the real part of the theoretical optical conductivity $\sigma_1^T(\omega)$ obtained by single-particle *ab initio* calculations of the FM ground state of $\text{Co}_3\text{Sn}_2\text{S}_2$ (see the Drude components over a broader range of the $\sigma_1(\omega)$ in Fig. S2a). The cut-off energy ω_c is usually chosen as the energy position where $\sigma_1(\omega)$ reaches its minimum below the interband transition, so the $\sigma_1^E(\omega, T = 8$ K) and the $\sigma_1^T(\omega)$ here have the cut-off energies $\omega_c^{8K} \approx 19.9$ meV and $\omega_c^T \approx 38.9$ meV, respectively. Integrating the Drude components of the $\sigma_1^E(\omega, T = 8$ K) and the $\sigma_1^T(\omega)$ up to the cut-off energies $\omega_c^{8K} \approx 19.9$ meV and $\omega_c^T \approx 38.9$ meV yields approximately the spectral weights of the experimental and theoretical Drude components: $S^{8K} \approx 8.6 \times 10^5 \Omega^{-1} \text{cm}^{-2}$ and $S^T \approx 1.8 \times 10^6 \Omega^{-1} \text{cm}^{-2}$, respectively (see the red and blue points in Fig. 2b). Considering the linear relationship between the K and the S , which is shown in equation (1), we get the ratio between the experimental kinetic energy at $T = 8$ K and the theoretical kinetic energy: $K_{8K}^E/K^T = S^{8K}/S^T \approx 0.47$. As shown in Fig. 2c, the ratios K_{8K}^E/K^T deduced by the above two methods are distinctly smaller than unity—the kinetic-energy ratio in conventional metals (such as Ag and Cu) with quite weak effects of many-body interactions [72]. Here, the substantial reduction in the electronic kinetic energy compared with the K^T indicates that many-body interactions which have not

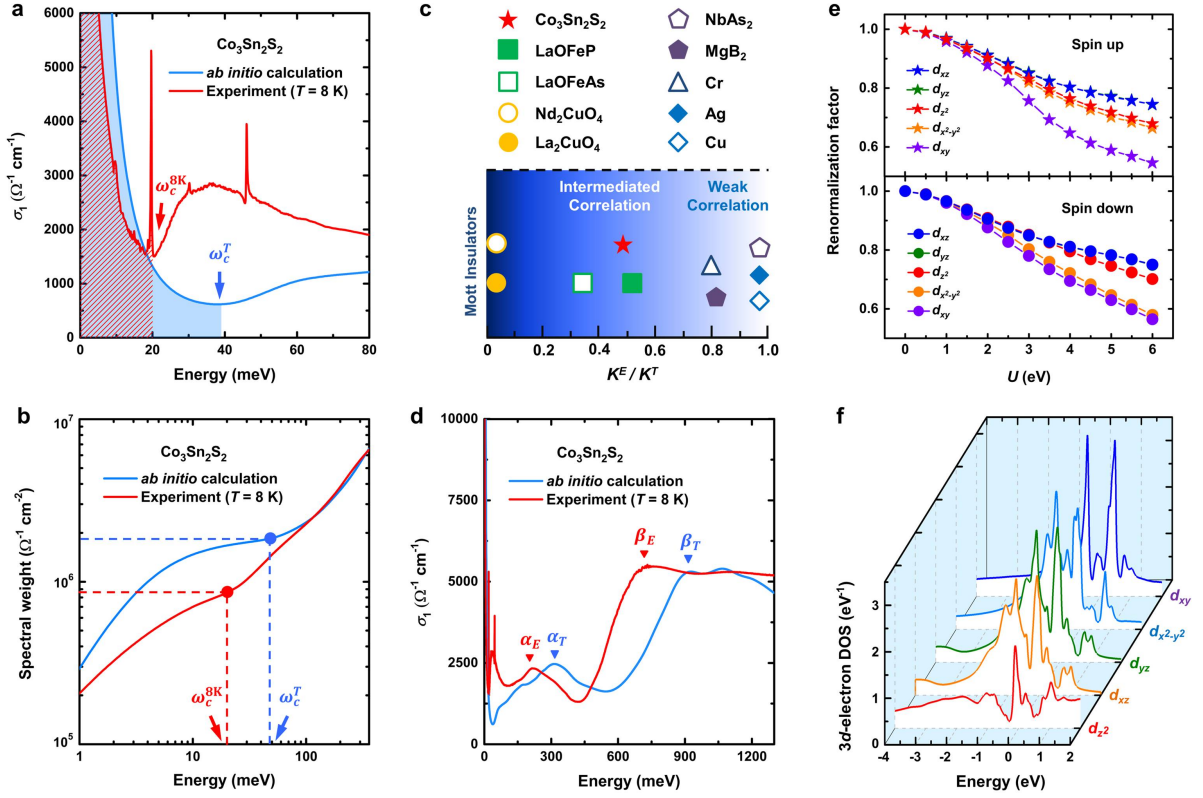


FIG. 2: **Electronic correlation effects in ferromagnetic $\text{Co}_3\text{Sn}_2\text{S}_2$.** **a**, Real parts of the experimental optical conductivity $\sigma_1^E(\omega)$ at temperature $T = 8$ K and the theoretical optical conductivity $\sigma_1^T(\omega)$ obtained by single-particle *ab initio* calculations. The cut-off energies (ω_c^{8K} and ω_c^T) for integrating the Drude components are chosen as the energy positions where the $\sigma_1^E(\omega, T = 8$ K) and the $\sigma_1^T(\omega)$ reach the minimum, respectively. **b**, Spectral weights of the $\sigma_1^E(\omega, T = 8$ K) at ω_c^{8K} and the $\sigma_1^T(\omega)$ at ω_c^T . **c**, Ratio of the experimental kinetic energy at $T = 8$ K and theoretical kinetic energy K_{8K}^E/K^T for $\text{Co}_3\text{Sn}_2\text{S}_2$ and several other quantum materials. The values of the K^E and K^T for other quantum materials can be gained from the following references: LaOFeP (Ref. [66]), LaOFeAs (Ref. [68]), topological nodal-line semimetal NbAs_2 (Ref. [70]), paramagnetic Cr (Ref. [71]), Ag (Ref. [72]), Cu (Ref. [72]), MgB_2 (Ref. [77]), Nd_2CuO_4 and La_2CuO_4 (Ref. [78]). **d**, Two interband-transition-induced peaks α_E and β_E in the $\sigma_1^E(\omega, T = 8$ K) and the two peaks α_T and β_T in the $\sigma_1^T(\omega)$. **e**, Coulomb-energy dependences of the electronic-bandwidth renormalization factors of the spin-up (upper panel) and spin-down (lower panel) Co 3d orbitals. The renormalization factors of the d_{xz} and d_{yz} orbitals are quite close to each other. **f**, Energy distributions of the 3d-electron density of states obtained by many-body calculations.

been taken into account by single-particle *ab initio* calculations have a pronounced effect of impeding the motion of the itinerant charge carriers in FM $\text{Co}_3\text{Sn}_2\text{S}_2$. In contrast, ordered spin-spin correlations in itinerant ferromagnets usually correspond to an increase in the kinetic energy of itinerant charge carriers [73], because (i) according to the Pauli exclusion principle, a larger kinetic energy is needed for the itinerant charge carriers with parallel spins to meet in the same lattice sites [74], and (ii) in the framework of the Stoner model, a phase transition from paramagnetism to itinerant ferromagnetism is accompanied with the increase in the electronic kinetic energy which is outweighed by the lowering of the exchange energy [75]. Thus, ordered spin-spin correlations in FM $\text{Co}_3\text{Sn}_2\text{S}_2$ are highly likely to be irrelevant with the remarkable reduction of the electronic kinetic energy here. Moreover, note that extremely strong electron-phonon coupling in a polar semiconductor or an ionic

crystal can lead to a significant reduction of the electronic kinetic energy owing to the formation of polarons [76]. Nevertheless, the calculated cobalt-3d-orbital-dominated bands which cross the E_F [37, 47–49] and the measured magnetic moment ($\sim 0.3 \mu_B/\text{Co}$) which is much smaller than the magnetic moment ($3 \mu_B/\text{Co}$) of isolated cobalt atoms [51–54] strongly suggest that FM $\text{Co}_3\text{Sn}_2\text{S}_2$ should not be a polar semiconductor or an ionic crystal, either of which has been found to host polarons. Generally, electron-phonon coupling in a material with the absence of polarons would not make the ratio between experimental and theoretical kinetic energies much smaller than unity (see the K^E/K^T in MgB_2 superconductor with electron-phonon mediated conventional superconductivity in Fig. 2c) [77, 78], so for FM $\text{Co}_3\text{Sn}_2\text{S}_2$, electron-phonon coupling is also unlikely to be the main factor causing the substantial decrease in its electronic kinetic energy. Based on the above discussion, electronic corre-

lations, which were previously revealed to result in the remarkable lowerings of the electronic kinetic energies in some transition-metal-based superconductors, such as the iron pnictides LaOFeP and LaOFeAs (see Fig. 2c) [66, 68], should play a dominant role in hampering the motion of the itinerant charge carriers in FM Co₃Sn₂S₂. Since the K_{8K}^E/K^T in FM Co₃Sn₂S₂ is approximately equal to the average of the kinetic-energy ratio (~ 0) in Mott insulators (like Nd₂CuO₄ and Sr₂CuO₄) with very strong electronic correlations (see Fig. 2c) and the kinetic-energy ratio (~ 1) in conventional metals (such as Ag and Cu) with quite weak electronic correlations, the strength of electronic correlations in FM Co₃Sn₂S₂ can be regarded to be intermediate.

Narrowness of the electronic bandwidth. To investigate the effect of many-body interactions on the electronic bandwidth of FM Co₃Sn₂S₂, we plotted the $\sigma_1^E(\omega)$, $T = 8$ K) and the $\sigma_1^T(\omega)$ over a broad energy range up to 1350 meV in Fig. 2d. The overall shape of the $\sigma_1^E(\omega)$ at $\omega > 20$ meV is quite similar to that of the $\sigma_1^T(\omega)$, but the energy positions of the two peak-like features arising from interband transitions, α_E at ~ 217.4 meV and β_E at ~ 708.1 meV, in the $\sigma_1^E(\omega)$, $T = 8$ K) are distinctly lower than those of the two corresponding peak-like features in the $\sigma_1^T(\omega)$, α_T at ~ 319.7 meV and β_T at ~ 931.6 meV. Since the energy of the interband-transition peak here is equal to the energy difference between the occupied and empty states in the electronic bands, the redshift of the two interband-transition-induced peaks in the experimental $\sigma_1^E(\omega)$, $T = 8$ K) compared with the two theoretical peaks in the $\sigma_1^T(\omega)$ indicates that many-body interactions have a significant effect of narrowing the electronic bandwidth of FM Co₃Sn₂S₂. Given that (i) according to the Pauli exclusion principle and the Stoner model, ferromagnetically ordered spin-spin correlations usually leads to a gain in the electronic kinetic energy [73–75], (ii) the gain in the electronic kinetic energy mostly corresponds to an extension of the electronic bandwidth [73–75], and (iii) the cut-off energy (~ 50.8 meV) of the phonon spectrum shown in Fig. 1f is much lower than the energies of the interband-transition-induced peaks, α_E , α_T , β_E , and β_T , ferromagnetically ordered spin-spin correlations and electron-phonon coupling are unlikely to be the leading interactions which cause the narrowing of the electronic bandwidth here. Therefore, electronic correlations in FM Co₃Sn₂S₂ ought to play a major part in narrowing the electronic bandwidth. To estimate the Coulomb-interaction strength U of electronic correlations in FM Co₃Sn₂S₂, we performed many-body calculations, i.e., combination of density functional theory and dynamical mean-field theory (DFT+DMFT) (see the details in Methods section) [79, 80], and then obtained the U dependences of the electronic-bandwidth renormalization factor quantifying the effect of electronic correlations on narrowing the electronic bandwidth (see Fig.

2e). The energy ratios between the experimental and theoretical peaks in Fig. 2d, $E(\alpha_E)/E(\alpha_T) \approx 0.68$ and $E(\beta_E)/E(\beta_T) \approx 0.76$, reflect the electronic-bandwidth renormalization effect of the electronic correlations with $U \sim 4$ eV, shown in Fig. 2e. Here, the difference in the two energy ratios may arise from the discrepancy between the renormalization factors of the five $3d$ orbitals (see Fig. 2e) and the difference between the energy distributions of the $3d$ -electron DOS gotten by DFT+DMFT calculations (see Fig. 2f).

Persistence of a Weyl semimetal state. To check whether a WSM state still exist in correlated Co₃Sn₂S₂, we carried out DFT+DMFT calculations with $U \sim 4$ eV to obtain its electronic surface and bulk states (see Methods section). In Fig. 3a, compared with the *ab-initio*-calculation-derived bulk bands (see the red dashed curves) along the high-symmetry lines of the Brillouin zone (see the upleft inset), the bulk momentum-resolved electronic spectra (see the bright yellow curves) gotten by DFT+DMFT calculations are indeed renormalized. In Fig. 3b, the Fermi-arc structures on the (001) surface, which are based on the quasiparticle bands from DFT+DMFT calculations, connect three pairs of Weyl points, respectively. Figure 3c depicts a pair of bulk Weyl cones along the direction (i.e., W_1 - W_2) connecting the Weyl points W_1 (i.e., blue point) and W_2 (i.e., red point) in Fig. 3b. To study the chirality of these two Weyl points W_1 and W_2 , we calculated the Berry curvature around each Weyl point. As displayed in Fig. 3d and 3e, W_1 and W_2 act as a source and a sink of Berry curvature, respectively, so W_1 and W_2 have opposite chirality [9–14]. The surface Fermi arc connecting each pair of Weyl points with opposite chirality and the bulk Weyl cones in FM Co₃Sn₂S₂, which were obtained by our DFT+DMFT calculations, indicate the existence of a WSM state in this magnetic system with intermediate-strength electronic correlations.

Flat band connecting the two Weyl cones. To further search for possible effects of intermediate-strength electronic correlations on the WSM state in FM Co₃Sn₂S₂, we derived its quasiparticle band structure along the direction W_1 - W_2 connecting the two Weyl points via DFT+DMFT calculations. The left panel of Fig. 4a shows that (i) a band B_0 obtained by single-particle *ab initio* calculations, which not only is a part of the two Weyl cones but also links the two Weyl cones, is turned into a flat band B_1 near E_F in the quasiparticle band structure by electronic correlations, and that (ii) two bands B_2 and B_3 , which have dispersionless parts and are absent along W_1 - W_2 in the single-particle band structure, emerges below E_F in the quasiparticle band structure. Since (i) the flat band B_1 and the dispersionless parts of bands B_2 and B_3 have divergent DOS (see the right panel of Fig. 4a) and (ii) optical absorptions

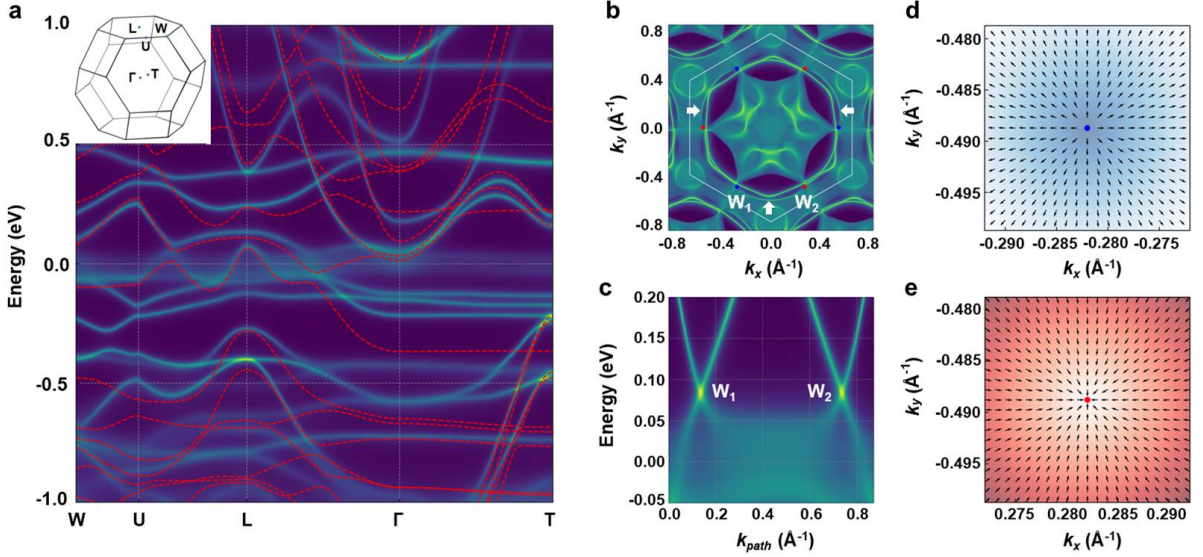


FIG. 3: **Many-body-calculation-derived electronic structure of ferromagnetic $\text{Co}_3\text{Sn}_2\text{S}_2$.** **a**, Momentum-resolved electronic spectra and single-particle band-structure along the high-symmetry lines of the bulk Brillouin zone (the upleft inset). The momentum-resolved electronic spectra are in bright yellow color. The single-particle band-structure is represented by the red dashed curves. **b**, Fermi arcs on the (001) surface. The blue and red dots, W_1 and W_2 , represent the projected Weyl points with positive and negative chirality, respectively. The three white arrows indicate the Fermi arcs. **c**, Bulk Weyl cones along the direction connecting the Weyl points W_1 and W_2 in **b**. **d,e**, Distribution of the Berry curvature around the Weyl points W_1 (**d**) and W_1 (**e**) in the k_{xy} plane.

are determined by the joint DOS of the initial and final state, the four interband transitions related to the flat band B_1 or the dispersionless part of band B_2 (or B_3), which are illustrated by the four colored arrows in the left panel of Fig. 4a, cause the four obvious peak-like features T_1 , T_2 , T_3 and T_4 around 38 meV, 70 meV, 113 meV and 131 meV in the real part of the optical conductivity $\sigma_1^{QP}(\omega)$ contributed by the direct optical transitions between the calculated quasiparticle bands, respectively (see the green spectrum Fig. 4b and the details on calculating the $\sigma_1^{QP}(\omega)$ in Methods section). Therein, (i) the strongest peak-like feature T_1 comes primarily from the optical transitions between the flat bands B_1 and the top of band B_2 (see the yellow arrow in Fig. 4a), and (ii) the second strongest peak-like feature T_2 arises mainly from the optical transitions between the flat band B_1 and the top of band B_3 (see the pink arrow in Fig. 4a). Considering that the present of the peak-like features T_1 and T_2 are intimately associated with the existence of the flat band B_1 , the peak-like features T_1 around 38 meV and T_2 around 70 meV can be regarded as two spectroscopic signatures of the existence of the flat band B_1 . It is worth noticing that the experimental $\sigma_1^E(\omega, T = 8 \text{ K})$ of FM $\text{Co}_3\text{Sn}_2\text{S}_2$ has an asymmetric peak-like feature around 36 meV, which can not be well reproduced by only one Lorentzian term in a standard Drude-Lorentz model [64–69]. By fitting the low-energy part of the $\sigma_1^E(\omega, T = 8 \text{ K})$ based on the Drude-Lorentz model, we find that this experimental peak-like feature can be decomposed into

four components: a Lorentzian peak with the strongest intensity around 36 meV, a Lorentzian peak with the second strongest intensity around 70 meV, a Lorentzian peak around 113 meV and a Lorentzian peak around 131 meV (see Methods section, the gray spectrum and the shaded peaks in Fig. 4b), which are consistent with the four peak-like features originating from the optical transitions related to the flat band B_1 or the dispersionless part of band B_2 (or B_3). Besides, this asymmetric peak-like feature in the experimental $\sigma_1^E(\omega, T = 8 \text{ K})$ becomes weaker as the temperature increases and disappears completely above the FM transition temperature (i.e., not in the WSM state) (see Fig. 1d), which is in agreement with the absence of the Weyl cones and the flat band connecting the Weyl cones above the FM transition temperature. Therefore, the experimental peak-like feature around 36 meV in the $\sigma_1^E(\omega, T = 8 \text{ K})$, which is obvious only in the FM state at low temperatures (i.e., in the WSM state) and includes the two Lorentzian peaks around the energy positions of T_1 and T_2 , provides spectroscopic evidence for the existence of the flat band B_1 near E_F in FM $\text{Co}_3\text{Sn}_2\text{S}_2$. Moreover, in stark contrast to the experimental $\sigma_1^E(\omega, T = 8 \text{ K})$ and the calculated $\sigma_1^{QP}(\omega)$, the interband-transition-contributed part of the $\sigma_1^T(\omega)$ obtained by single-particle *ab initio* calculations has no distinct peak-like feature around 38 meV (see Fig. 4b), which further supports that electronic correlations in FM $\text{Co}_3\text{Sn}_2\text{S}_2$ flatten the band linking the two Weyl cones and induce the emergence of the flat band B_1 .

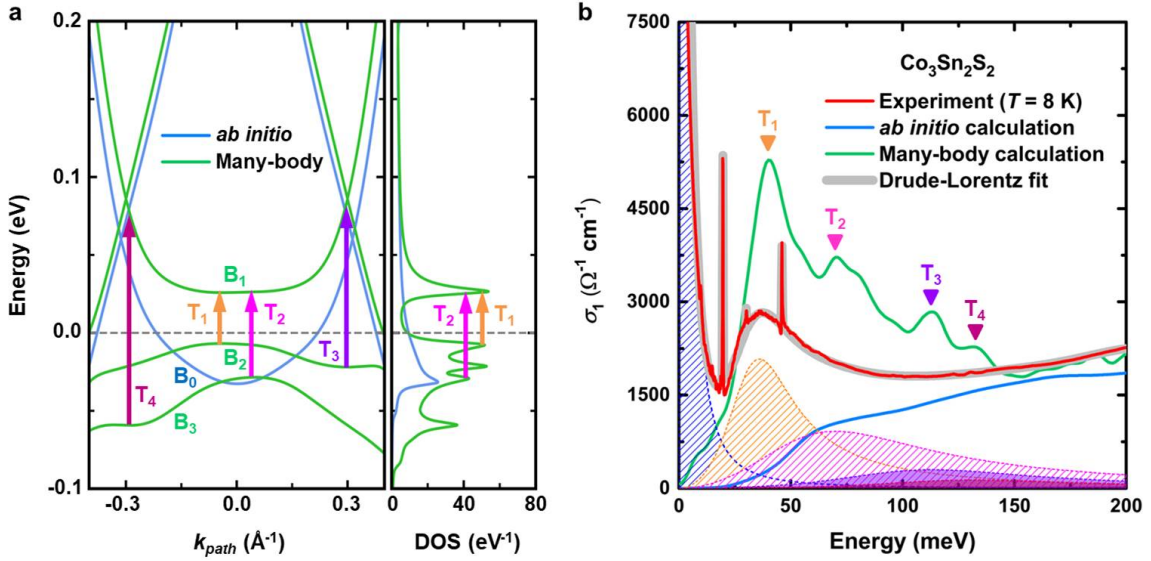


FIG. 4: **Flat band and related optical transitions in ferromagnetic $\text{Co}_3\text{Sn}_2\text{S}_2$.** **a**, Left panel: quasiparticle band structure obtained by many-body calculations (i.e., DFT+DMFT calculations) (green curve) and band structure gotten by single-particle *ab initio* calculations (blue curve) along the direction connecting the Weyl points. Right panel: density of states (DOS) of the quasiparticle bands. The four arrows in the left panel show the optical transitions related to the flat band B_1 or the dispersionless part of band B_2 (or B_3) with divergent DOS. **b**, Experimental and calculated real parts $\sigma_1(\omega)$ of the optical conductivity at low energies. Four peak-like features (T_1 , T_2 , T_3 and T_4) in the $\sigma_1(\omega)$ obtained by many-body calculations are present around 39 meV, 70 meV, 113 meV and 131 meV, respectively. These four peak-like features arise mainly from the four optical transitions illustrated by the four arrows in **a**. The asymmetric peak-like feature around 36 meV in the experimental $\sigma_1(\omega)$ at $T = 8$ K can be fitted with the four Lorentzian peaks (see the shaded peaks in **b**), which are located around 36 meV, 70 meV, 113 meV and 131 meV, respectively. Peak-like feature is absent around 38 meV in the interband-transition-contributed part of the $\sigma_1^T(\omega)$ obtained by single-particle *ab initio* calculations (see the blue spectrum in **b**).

Discussion

In summary, we have investigated electronic correlations in a magnetic WSM candidate $\text{Co}_3\text{Sn}_2\text{S}_2$. The electronic kinetic energy extracted from the measured optical data is about half of that deduced by single-particle *ab initio* calculations, which indicates that the strength of electronic correlations in $\text{Co}_3\text{Sn}_2\text{S}_2$ is intermediate. In addition, the energies of the two interband-transition peaks in the experimental $\sigma_1^E(\omega, T = 8 \text{ K})$ of $\text{Co}_3\text{Sn}_2\text{S}_2$ are significantly lower than those in the $\sigma_1^T(\omega)$ obtained by single-particle *ab initio* calculations, which manifests that its electronic bandwidth is narrowed by electronic correlations. Furthermore, by comparing the energy ratios between the interband-transition peaks in the experimental and single-particle-*ab-initio*-calculation-derived real parts of the optical conductivity with the electronic-bandwidth renormalization factors gotten by DFT+DMFT calculations, we estimated the Coulomb-interaction strength ($U \sim 4 \text{ eV}$) of electronic correlations in this material. Our DFT+DMFT calculations with $U \sim 4 \text{ eV}$ show that a WSM state still exists in this correlated system. Besides, the consistence between the asymmetric peak-like feature around 36 meV in the experimental $\sigma_1^E(\omega, T = 8 \text{ K})$ and the DFT+DMFT-calculation-derived peak-like features in the $\sigma_1^{QP}(\omega)$ reveals an electronic band connecting the two Weyl cones

is flattened by electronic correlations and is present near E_F in FM $\text{Co}_3\text{Sn}_2\text{S}_2$. Our results not only show that FM $\text{Co}_3\text{Sn}_2\text{S}_2$ is an electron-correlated WSM, but also open an avenue for deeply investigating exotic quantum phenomena dominated by flat bands in WSMs.

Methods

Optical reflectance measurements. The optical reflectance measurements in the energy range from 8 to 6000 meV were performed on a Bruker Vertex 80v Fourier-transform spectrometer. The single-crystal sample was mounted on an optically black cone locating at the cold finger of a helium flow cryostat. A freshly-cleaved *ab*-plane of the $\text{Co}_3\text{Sn}_2\text{S}_2$ single crystal was obtained just before pumping the cryostat. An *in situ* gold and aluminum overcoating technique was employed to get the reflectance spectra $R(\omega)$. The optical reflectance data are highly reproducible. Moreover, J. A. Woollam RC2 spectroscopic ellipsometer was used to get the optical constants of the $\text{Co}_3\text{Sn}_2\text{S}_2$ single crystals in the energy range from 500 to 6000 meV, which are consistent with the optical constants extracted from the measured reflectance spectra in this energy range.

Single-crystal growth. The $\text{Co}_3\text{Sn}_2\text{S}_2$ single crystals were grown by a self-flux method. High-purity elemental

Co, Sn and S with a molar ratio of 3:2:2 were put into an alumina crucible and then sealed in a quartz tube under high vacuum. The quartz tube was slowly heated to 637 K and maintained for two days due to the high vapor pressure of sulfur. Afterwards, the quartz tube was heated to 1273 K within 10 hours and then slowly cooled down to 973 K before switching off the furnace. Shining crystal faces can be obtained by cleaving the $\text{Co}_3\text{Sn}_2\text{S}_2$ single crystals.

Kramers-Kronig transformation. The $\sigma_1(\omega)$ were obtained by the Kramers-Kronig transformation of the $R(\omega)$. A Hagen-Rubens relation was used for low-energy extrapolation, and a $\omega^{-0.15}$ dependence was used for high-energy extrapolation up to 80000 meV, above which a ω^{-4} dependence was employed. The reciprocal value of the obtained $\sigma_1(\omega) = 0$ at each temperature coincides with the direct current resistivity obtained by the transport measurements (see Fig. S2b of Supplementary Information), which indicates that the Kramers-Kronig transformation of the $R(\omega)$ here is reliable.

Calculating the scattering rate spectra. The scattering rate spectra $1/\tau(\omega)$ can be obtained by performing the extended Drude analysis of the optical data according to equation (9) in Ref. [64]:

$$1/\tau(\omega) = \frac{2\pi\omega_p^2}{Z_0} \text{Re} \left(\frac{1}{\sigma(\omega)} \right) = \frac{2\pi\omega_p^2}{Z_0} \frac{\sigma_1(\omega)}{\sigma_1^2(\omega) + \sigma_2^2(\omega)}, \quad (2)$$

where $Z_0 \approx 377 \Omega$ is the impedance of free space, ω_p is the plasma frequency, $\sigma(\omega)$ is the complex optical conductivity, $\sigma_1(\omega)$ is the real part of the $\sigma(\omega)$ and $\sigma_2(\omega)$ is the imaginary part of the $\sigma(\omega)$. The $\sigma_1(\omega)$ and $\sigma_2(\omega)$ can be deduced by the Kramers-Kronig transformation of the measured $R(\omega)$.

Single-particle *ab initio* calculations. Our single-particle *ab initio* optical conductivity calculations were performed by using the full potential linearized augmented plane wave method implemented in the WIEN2k package [81]. The k -point mesh for the Brillouin zone integration is $36 \times 36 \times 36$, and the plane wave cut-off K_{max} is given by $R_{mt} * K_{max} = 8.0$. The spin-orbit coupling effects are included in our calculations. The phonon dispersions were calculated by using the open source code PHONOPY [82]. The phonon force constants in real space were calculated based on the density-functional perturbation theory (DFPT) method using Vienna *ab initio* simulation package (VASP) [83] with a $2 \times 2 \times 2$ supercell. The plane wave energy cut-off was chosen as 400 eV, and a Γ -centered k -point grid with $3 \times 3 \times 3$ discretization was used.

Many-body calculations. The method of density functional theory plus dynamical mean field theory (DFT+DMFT) can capture dynamic quantum fluctuation effects and thus is suitable for investigating the quasiparticles in correlated metals, while DFT+ U method is a static Hatree-Fock approach (see the band

structures of $\text{Co}_3\text{Sn}_2\text{S}_2$ obtained by DFT+ U calculations in Fig. S5 and Supplemental section II of Supplementary Information). The correlated electronic structure of $\text{Co}_3\text{Sn}_2\text{S}_2$ was obtained by DFT+DMFT calculations. A Wannier tight binding (TB) Hamiltonian consisting of $3d$ orbitals of the three Co atoms, and p orbitals of the two Sn atoms and the two S atoms was constructed using the Wannier90 package [84]. The hybridization between the d orbitals and the p orbitals, together with the spin-orbit coupling effect, is included in our model. Only $3d$ electrons in Co are treated as correlated ones in DFT+DMFT calculations. We chose the fully localized form $\Sigma_{DC} = U(n_d^0 - \frac{1}{2}) - \frac{1}{2}J(n_d^0 - 1)$, where n_d^0 is nominal occupation of $3d$ orbitals, as the “double-counting” scheme.

We used the hybridization expansion version of the continuous-time quantum Monte Carlo (HYB-CTQMC) method implemented in the iQIST package [85, 86] as the impurity solver. The local on-site Coulomb interactions are parameterized by the Slater integrals F^0 , F^2 and F^4 . Hubbard U and Hund’s coupling J amount to $U = F^0$, $J = (F^2 + F^4)/14$. The constrained DFT calculations suggest $U = 5.1$ eV and $J = 0.9$ eV for Co^{2+} in CoO [87]. Besides, the experimental optical absorption data indicate $J_H \approx 0.8$ eV [88]. Thus, in order to check the effective U and J related to the renormalization factor Z , we fixed the ratio of $J/U = 0.2$ to change U , which was also used in d^7 cobalt compounds study [89]. We only keep the density-density terms of the Coulomb interactions for computational efficiency. The inverse temperature is $\beta = 1/(K_B T) = 40$ eV $^{-1}$. The standard deviation of the self-energy is less than 0.03 in the last self-consistent loop. We used the analytical continuation method introduced by K. Haule [90] to extract the self-energy $\Sigma(\omega)$ on real axis from the Matsubara self-energy $\Sigma(i\omega)$ obtained from CTQMC.

In order to study the topological electronic structure of $\text{Co}_3\text{Sn}_2\text{S}_2$, we calculated the momentum-resolved spectra, which is defined as

$$A(k, \omega) = -\frac{1}{\pi} \Im \left[\frac{1}{\omega + \mu - H_0(k) - \tilde{\Sigma}(k, \omega)} \right] \quad (3)$$

where, $H_0(k)$ is the non-interaction Hamiltonian at each k -point from DFT calculation, $\tilde{\Sigma}(k, \omega) = \hat{P}_k(\Sigma(\omega) - \Sigma_{dc})$, \hat{P}_k are the projection operators.

The low-energy quasiparticle (QP) behaviour is described by the following QP Hamiltonian,

$$H_{QP} = H_0 - \mu + \Re \tilde{\Sigma}(0) \quad (4)$$

Our (001) surface electronic structure, Fermi arcs and Berry curvature were calculated based on the low-energy QP Hamiltonian. The surface spectra (i.e., Fermi arcs) were calculated by using the iterative Green’s function method [91] as implemented in the WannierTools package [92].

The real part of the optical conductivity $\sigma_1^{QP}(\omega)$ contributed by the direct optical transitions between the calculated quasiparticle bands in the main text was calculated by the Kubo-Greenwood formula as implemented in the Wannier90 package [64, 69, 84].

Fitting based on the Drude-Lorentz model. We fit the $\sigma_1^E(\omega, T = 8 \text{ K})$ of $\text{Co}_3\text{Sn}_2\text{S}_2$ using a standard Drude-Lorentz model [64–69]:

$$\sigma_1(\omega) = \frac{2\pi}{Z_0} \frac{\omega_D^2 \Gamma_D}{\omega^2 + \Gamma_D^2} + \sum_{j=1}^N \frac{2\pi}{Z_0} \frac{S_j^2 \omega^2 \Gamma_j}{(\omega_j^2 - \omega^2)^2 + \omega^2 \Gamma_j^2}, \quad (5)$$

where $Z_0 \approx 377 \Omega$ is the impedance of free space, ω_D is the plasma frequency, and Γ_D is the relaxation rate of itinerant charge carriers, while ω_j , Γ_j and S_j are the resonance frequency, the damping, and the mode strength of each Lorentz term, respectively. The first term in Eq. (5) denotes the optical response of free carriers, i.e., Drude response. The Lorentzian terms can describe the contributions from inter-band transitions. The parameters of the four Lorentzian terms and the Drude term for fitting the low-energy part of the $\sigma_1^E(\omega, T = 8 \text{ K})$ are listed in Table I.

TABLE I: Parameters of the Lorentzian and Drude terms

j	ω_j (meV)	Γ_j (meV)	S_j (meV)	ω_D (meV)	Γ_D (meV)
1	36	37	214	–	–
2	70	98	231	–	–
3	113	108	139	–	–
4	131	108	92	–	–
D	–	–	–	258	2.5

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Author contributions

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Competing financial interests

The authors declare no competing financial interests.